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Non-Equilibrium Steady States

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Abstract

The mathematical physics of mechanical systems in thermal equilibrium is a well studied, and relatively easy, subject, because the Gibbs distribution is in general an adequate guess for the equilibrium state.

On the other hand, the mathematical physics of *non-equilibrium* systems, such as that of a chain of masses connected with springs to two (infinite) heat reservoirs is more difficult, precisely because no such *a priori* guess exists.

Recent work has, however, revealed that under quite general conditions, such states can not only be shown to exist, but are *unique*, using the Hörmander conditions and controllability. Furthermore, interesting properties, such as energy flux, exponentially fast convergence to the unique state, and fluctuations of that state have been successfully studied.

Finally, the ideas used in these studies can be extended to certain stochastic PDE's using Malliavin calculus to prove regularity of the process.

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1. The Model and Results

I report here on work done, in different combinations, together with *Martin Hairer, Luc Rey-Bellet, Claude-Alain Pillet, and Lawrence Thomas*. In it, we considered the seemingly trivial problem of describing the non-equilibrium statistical mechanics of a finite-dimensional non-linear Hamiltonian system coupled to two infinite heat reservoirs which are at *different* temperatures. By this I mean that the stochastic forces of the two heat reservoirs differ. The difficulties in such a problem are related to the absence of an easy *a priori* estimate for the state of the system. We show under certain conditions on the initial data that the system goes to a *unique* non-equilibrium steady state and we describe rather precisely some properties of this steady state. These are,

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- appearance of an energy flux (from the hot to the cold reservoir) whenever the reservoirs are at different temperatures,
- exponential stability of this state,
- fluctuations around this state satisfy the Cohen-Gallavotti fluctuation conjecture.

I first review the construction of the model. Two features need special attention: The modeling of the heat reservoirs and their coupling to the chain, and the nature of the coupling among the masses in the chain. I start with the latter: It is a 1-dimensional chain of n distinct d-dimensional anharmonic oscillators with nearest neighbor coupling. The phase space of the chain is therefore $\mathbf{R}^{2dn}$ and its dynamics is described by a $\mathcal{C}^\infty$ Hamiltonian function of the form

$$H_{\rm S}(p,q) \;=\; \sum_{j=1}^{n} \frac{p_j^2}{2} + \sum_{j=1}^{n} U_j^{(1)}(q_j) + \sum_{i=1}^{n-1} U_i^{(2)}(q_i - q_{i+1}) \;\equiv\; \sum_{j=1}^{n} \frac{p_j^2}{2} + V(q)\ , \quad (1.1)$$

where $q=(q_1,\dots,q_n)$, $p=(p_1,\dots,p_n)$, with $p_i,\, q_i \in \mathbf{R}^d$. We will eventually couple the ends of the chain, *i.e.*, q_1 and q_n, to heat reservoirs. Clearly, for heat conduction to be possible at all we must require that the $U_i^{(2)}$ are non-zero. But, this is not enough and the interaction has to have a minimal strength. A sufficient condition for the main result to hold is: For some $m_2 \ge m_1 \ge 2$, and all sufficiently large $|q|$, we require

$$0 \,<\, c_1 \,\le\, \frac{U_i^{(1)}(q)}{(1+|q|)^{m_1}} \,\le\, c_1'\ , \qquad 0 \,<\, c_2 \,\le\, \frac{U_i^{(2)}(q)}{(1+|q|)^{m_2}} \,\le\, c_2'\ ,$$

and similar growth conditions on the first and second derivatives. Finally, we require that each of the $(d\times d)$ matrices

$$\nabla_{q_i}\nabla_{q_{i+1}} U_i^{(2)}(q_i - q_{i+1})\ , \quad i = 1,\dots,n-1\ , \qquad (1.2)$$

is non-degenerate (see [12] for the most general conditions).

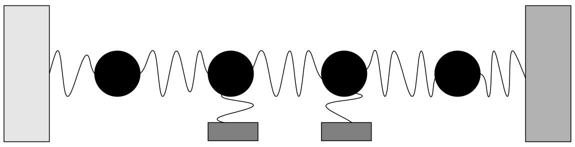

Fig. 1: Model of the chain with the two reservoirs at its ends, "Hot" at left, "Cold" at right.

Remark 1.1. It seems that relaxing the condition (1.2) poses hard technical problems, although, from a physical point of view, allowing the matrix to be degenerate on hyper-surfaces of codimension ≥ 1 should work. See [9,12] for some possibilities.

Remark 1.2. If $m_2 < m_1$ it seems that the existence of a unique state is jeopardized by the potential appearance of breathers. Indeed, too much energy can then be "stored" in $U^{(1)}$ without being sufficiently "transported" between the oscillators. A more detailed understanding of this problem would be welcome.

Remark 1.3. The nature of the steady state in the limit of an infinite chain ($n \to \infty$) is a difficult open question.

As a model of a heat reservoir we consider the classical field theory associated with the d-dimensional wave equation. The field φ and its conjugate momentum field π are elements of the real Hilbert space $\mathcal{H} = \mathrm{H}^1_{\mathbf{R}}(\mathbf{R}^d) \oplus \mathrm{L}^2_{\mathbf{R}}(\mathbf{R}^d)$ which is the completion of $\mathcal{C}_0^\infty(\mathbf{R}^d) \oplus \mathcal{C}_0^\infty(\mathbf{R}^d)$ with respect to the norm defined by the scalar product:

$$\left(\begin{pmatrix} \varphi \\ \pi \end{pmatrix}, \begin{pmatrix} \varphi \\ \pi \end{pmatrix} \right)_{\mathcal{H}} = \int \mathrm{d}x \, \left(|\nabla\varphi(x)|^2 + |\pi(x)|^2 \right) \equiv 2H_{\mathrm{B}}(\varphi, \pi) \,, \tag{1.3}$$

where H_{B} is the Hamiltonian of a bath and the corresponding equation of motion is the ordinary wave equation which we write in the form

$$\begin{pmatrix} \dot\varphi(t) \\ \dot\pi(t) \end{pmatrix} = \mathcal{L} \begin{pmatrix} \varphi \\ \pi \end{pmatrix} \equiv \begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix} \begin{pmatrix} \varphi \\ \pi \end{pmatrix} .$$

Finally, we define the coupling between the chain and the heat reservoirs. The reservoirs will be called "L" and "R", the left one coupling to the coordinate q_1 and the right one coupling to the other end of the chain (q_n). Since we consider two heat reservoirs, the phase space of the coupled system, for finite energy configurations, is $\mathbf{R}^{2dn} \times \mathcal{H} \times \mathcal{H}$ and its Hamiltonian will be chosen as

$$\begin{aligned} H(p,q,\varphi_{\mathrm{L}},\pi_{\mathrm{L}},\varphi_{\mathrm{R}},\pi_{\mathrm{R}}) &= H_{\mathrm{S}}(p,q) + H_{\mathrm{B}}(\varphi_{\mathrm{L}},\pi_{\mathrm{L}}) + H_{\mathrm{B}}(\varphi_{\mathrm{R}},\pi_{\mathrm{R}}) \\ &\quad + q_1 \cdot \int \mathrm{d}x \, \varrho_{\mathrm{L}}(x) \nabla\varphi_{\mathrm{L}}(x) + q_n \cdot \int \mathrm{d}x \, \varrho_{\mathrm{R}}(x) \nabla\varphi_{\mathrm{R}}(x) \,. \end{aligned} \tag{1.4}$$

Here, the $\varrho_i(x) \in \mathrm{L}^1(\mathbf{R}^d)$ are charge densities which we assume for simplicity to be spherically symmetric functions. The choice of the Hamiltonian (1.4) is motivated by the dipole approximation of classical electrodynamics. We use the shorthand

$$\phi_i \equiv \begin{pmatrix} \varphi_i \\ \pi_i \end{pmatrix} .$$

We set $\alpha_i = \left(\alpha_i^{(1)}, \ldots, \alpha_i^{(d)}\right)$, $i \in \{\mathrm{L}, \mathrm{R}\}$, with

$$\widehat{\alpha}_i^{(\nu)}(k) \equiv \begin{pmatrix} -ik^{(\nu)}\widehat{\varrho}_i(k)/k^2 \\ 0 \end{pmatrix} .$$

The "hat" means the Fourier transform $\widehat{f}(k) \equiv (2\pi)^{-d/2} \int \mathrm{d}x \, f(x) e^{-ik\cdot x}$. With this notation the Hamiltonian is

$$H(p,q,\phi_{\mathrm{L}},\phi_{\mathrm{R}}) = H_{\mathrm{S}}(p,q) + H_{\mathrm{B}}(\phi_{\mathrm{L}}) + H_{\mathrm{B}}(\phi_{\mathrm{R}}) + q_1 \cdot (\phi_{\mathrm{L}}, \alpha_{\mathrm{L}})_{\mathcal{H}} + q_n \cdot (\phi_{\mathrm{R}}, \alpha_{\mathrm{R}})_{\mathcal{H}} \,,$$

where $H_{\mathrm{B}}(\phi)=\frac{1}{2}\|\phi\|_{\mathcal{H}}^2$. The equations of motions take the form

$$\begin{aligned}
\dot q_j(t) &= p_j(t)\ , \qquad j=1,\dots,n\ ,\\
\dot p_1(t) &= -\nabla_{q_1}V(q(t))-(\phi_{\mathrm{L}}(t),\alpha_{\mathrm{L}})_{\mathcal{H}}\ ,\\
\dot p_j(t) &= -\nabla_{q_j}V(q(t))\ , \qquad j=2,\dots,n-1\ ,\\
\dot p_n(t) &= -\nabla_{q_n}V(q(t))-(\phi_{\mathrm{R}}(t),\alpha_{\mathrm{R}})_{\mathcal{H}}\ ,\\
\dot\phi_{\mathrm{L}}(t) &= \mathcal{L}\left(\phi_{\mathrm{L}}(t)+\alpha_{\mathrm{L}}\cdot q_1(t)\right)\ ,\\
\dot\phi_{\mathrm{R}}(t) &= \mathcal{L}\left(\phi_{\mathrm{R}}(t)+\alpha_{\mathrm{R}}\cdot q_n(t)\right)\ .
\end{aligned}\tag{1.5}$$

The last two equations of (1.5) are easily integrated and lead to

$$\begin{aligned}
\phi_{\mathrm{L}}(t) &= e^{\mathcal{L}t}\phi_{\mathrm{L}}(0)+\int_0^t \mathrm{d}s\,\mathcal{L}e^{\mathcal{L}(t-s)}\alpha_{\mathrm{L}}\cdot q_1(s)\ ,\\
\phi_{\mathrm{R}}(t) &= e^{\mathcal{L}t}\phi_{\mathrm{R}}(0)+\int_0^t \mathrm{d}s\,\mathcal{L}e^{\mathcal{L}(t-s)}\alpha_{\mathrm{R}}\cdot q_n(s)\ ,
\end{aligned}$$

where the $\phi_i(0)$, $i\in\{\mathrm{L},\mathrm{R}\}$, are the initial conditions of the heat reservoirs.

We next assume that the two reservoirs are in thermal equilibrium at inverse temperatures β_{L} and β_{R}. By this I mean that the initial conditions $\Phi(0)\equiv\{\phi_{\mathrm{L}}(0),\phi_{\mathrm{R}}(0)\}$ are random variables distributed according to a Gaussian measure with mean zero and covariance $\langle\phi_i(f)\phi_j(g)\rangle=\delta_{ij}(1/\beta_i)(f,g)_{\mathcal{H}}$. If we assume that the coupling functions $\alpha_i^{(\nu)}$ are in $\mathcal{H}$ for $i\in\{\mathrm{L},\mathrm{R}\}$ and $\nu\in\{1,\dots,d\}$, then the $\xi_i(t)\equiv\phi_i(0)(e^{-\mathcal{L}t}\alpha_i)$ are d-dimensional Gaussian random processes with mean zero and covariance

$$\langle\,\xi_i(t)\xi_j(s)\rangle \;=\; \delta_{i,j}\frac{1}{\beta_i}C_i(t-s)\ ,\quad i,j\in\{\mathrm{L},\mathrm{R}\}\ ,\tag{1.6}$$

where the $d\times d$ matrices $C_i(t-s)$ are

$$C_i^{(\mu,\nu)}(t-s) \;=\; \left(\alpha_i^{(\mu)},e^{\mathcal{L}(t-s)}\alpha_i^{(\nu)}\right)_{\mathcal{H}} \;=\; \frac{1}{d}\delta_{\mu,\nu}\int \mathrm{dk}\,|\widehat{\varrho}_i(k)|^2\cos\bigl(|k|(t-s)\bigr)\ .$$

Finally, we impose a condition on the random force exerted by the heat reservoirs on the chain. We assume that the covariances of the random processes $\xi_i(t)$ with $i\in\{\mathrm{L},\mathrm{R}\}$ satisfy

$$C_i^{(\mu,\nu)}(t-s) \;=\; \delta_{\mu,\nu}\lambda_i^2e^{-\gamma_i|t-s|}\ ,\tag{1.7}$$

with $\gamma_i>0$ and $\lambda_i>0$, which can be achieved by a suitable choice of the coupling functions $\varrho_i(x)$, for example

$$\widehat{\varrho}_i(k) \;=\; \text{const.}\prod_{m=1}^{M}\frac{1}{(k^2+\gamma_i^2)^{1/2}}\ ,\tag{1.8}$$

where all the γ_i are distinct. We continue with the case $M = 1$ for simplicity.

Using (1.7) and enlarging the phase space with auxiliary fields r_i, one eliminates the memory terms (both deterministic and random) of the equations of motion and rewrites them as a system of *Markovian* stochastic differential equations:

$$\begin{aligned}
\mathrm{d}q_j(t) &= p_j(t)\mathrm{d}t\ , \qquad\qquad j = 1, \dots, n\ ,\\
\mathrm{d}p_1(t) &= -\nabla_{q_1} V(q(t))\mathrm{d}t + r_{\mathrm{L}}(t)\mathrm{d}t\ ,\\
\mathrm{d}p_j(t) &= -\nabla_{q_j} V(q(t))\mathrm{d}t\ , \qquad j = 2, \dots, n-1\ ,\\
\mathrm{d}p_n(t) &= -\nabla_{q_n} V(q(t))\mathrm{d}t + r_{\mathrm{R}}(t)\mathrm{d}t\ ,\\
\mathrm{d}r_{\mathrm{L}}(t) &= -\gamma_{\mathrm{L}} r_{\mathrm{L}}(t)\mathrm{d}t + \lambda_{\mathrm{L}}^2\gamma_{\mathrm{L}}\ q_1(t)\mathrm{d}t - \lambda_{\mathrm{L}}\sqrt{2\gamma_{\mathrm{L}}\ /\beta_{\mathrm{L}}}\ \mathrm{d}w_{\mathrm{L}}(t)\ ,\\
\mathrm{d}r_{\mathrm{R}}(t) &= -\gamma_{\mathrm{R}} r_{\mathrm{R}}(t)\mathrm{d}t + \lambda_{\mathrm{R}}^2\gamma_{\mathrm{R}} q_n(t)\mathrm{d}t - \lambda_{\mathrm{R}}\sqrt{2\gamma_{\mathrm{R}}/\beta_{\mathrm{R}}}\,\mathrm{d}w_{\mathrm{R}}(t)\ ,
\end{aligned} \tag{1.9}$$

which defines a Markov diffusion process on $\mathbf{R}^{d(2n+2)}$.

Theorem 1.4. [3,4,12,1] *There is a constant $\lambda^* > 0$, such that when $|\lambda_{\mathrm{L}}|$, $|\lambda_{\mathrm{R}}| \in (0, \lambda^*)$, the solution of (1.9) is a Markov process which has an absolutely continuous invariant measure μ with a $\mathcal{C}^\infty$ density m. This measure is* **unique**, **mixing** *and attracts any other measure at an exponential rate.*

Remark 1.5. On can show even a little more. Let $h_0(\beta)$ be the Gibbs distribution for the case where both reservoirs are at temperature $1/\beta$. If h denotes the density of the invariant measure found in Theorem 1.4, we find that $h/h_0(\beta)$ is in the Schwartz space $\mathcal{S}$ for all $\beta < \min(\beta_{\mathrm{L}}, \beta_{\mathrm{R}})$. This mathematical statement reflects the intuitively obvious fact that the chain can not get hotter than either of the reservoirs.

Remark 1.6. The restriction on the couplings λ_{L}, λ_{R} between the small system and the reservoirs is a condition of stability (against "explosion") of the small system coupled to the heat reservoirs: It is *not* of perturbative nature. Indeed, the reservoirs have the effect of renormalizing the deterministic potential seen by the small system and this potential must be stable. This restricts λ_{L} and λ_{R}.

The proof of Theorem 1.4 is based on a detailed study of Eq.(1.9). Let $x = (p, q, r)$ and $r = (r_{\mathrm{L}}, r_{\mathrm{R}})$. For a Markov process $x(t)$ with phase space X and an invariant measure $\mu(\mathrm{d}x)$, ergodic properties may be deduced from the study of the associated semi-group T^t on the Hilbert space $\mathrm{L}^2(X, \mu(\mathrm{d}x))$. To prove the existence of the invariant measure in Theorem 1.4 one proceeds as follows: Consider first the semi-group T^t on the auxiliary Hilbert space $\mathcal{H}_0 \equiv \mathrm{L}^2(X, \mu_0(\mathrm{d}x))$, where the reference measure $\mu_0(\mathrm{d}x)$ is a generalized Gibbs state for a suitably chosen reference temperature. Our main technical result consists in proving that the generator L of the semi-group T^t on $\mathcal{H}_0$ and its adjoint have compact resolvent. This is proved by generalizing Hörmander's techniques for hypoelliptic operators of "Kolmogorov type" to the problem in unbounded domains described by (1.9). Once this is established, we deduce the existence of a solution to the eigenvalue equation $(T^t)^* g = g$ in $\mathcal{H}_0$ and this implies immediately the existence of an invariant measure. The original proof [3] was subsequently improved by using more probabilistic techniques [12].

The proof of uniqueness, [4], relies on global controllability of (1.9). In it, one shows that the control equation, in which the noises w_i of (1.9) are replaced by deterministic forces f_i (in the same function space), allows one to reach any given point in phase space in any prescribed time, by choosing the forces f_i adequately. It is here that, at least at the time of this writing, a feature of the problem seems crucial for success:

Remark 1.7. The geometry of the chain: If the chain is not of linear geometry, but with parallel strands, or if the coupling is not of pure nearest neighbor type, uniqueness of the invariant measure does in general not follow from the methods described here. Very simple counterexamples with harmonic chains [14] show that this problem is not easy.

Remark 1.8. We proved in [3, Lemma 3.7] that the density $\varrho = \varrho_T$ is a real analytic function of $\zeta = (T_{\rm L} - T_{\rm R})/(T_{\rm L} + T_{\rm R})$. In particular, this yields the standard perturbative results near equilibrium ($\zeta = 0$).

Question. A fascinating problem is to understand the limit of a chain of infinitely many oscillators, and in particular the nature of heat conduction in this case. I believe that this problem can only be solved if a better understanding of modeling the coupling between the heat bath and the chain can be found.

2. Time-Reversal, Energy Flux, and Entropy Production

In the wake of the seminal work of Gallavotti and Cohen [6], several authors realized (*e.g.*, [10, 11]) that internal symmetries of stationary non-equilibrium problems lead to an interesting relation for the fluctuations in the stationary state. The model we consider here is no exception, and it is one of the few examples where the Hamiltonian dynamics plays a very nice role.

It will be useful to streamline the notation.[1] The two reservoirs, L and R, are described by the variables $r = (r_{\rm L}, r_{\rm R}) \in \mathbf{R}^d \oplus \mathbf{R}^d$. Let Λ be the $(2d \times nd)$ matrix defined by

$$q \cdot \Lambda r \;=\; q_1 \cdot \Lambda_{\rm L} r_{\rm L} + q_n \cdot \Lambda_{\rm R} r_{\rm R} \;=\; q_1 \lambda_{\rm L} r_{\rm L} + q_n \lambda_{\rm R} r_{\rm R} \;.$$

Define the $(2d \times 2d)$ matrix $\Gamma = \operatorname{diag} \gamma_{\rm L} \oplus \operatorname{diag} \gamma_{\rm R}$, let $w = w_{\rm L} \oplus w_{\rm R}$ the $2d$-dimensional standard Brownian motion, and finally T the (2×2) diagonal temperature matrix $T = \operatorname{diag}(T_{\rm L}, T_{\rm R})$. It is useful to introduce the change of variables

[1] This notation generalizes more easily to the case $M > 1$ of (1.8) .

$s = Fr - F^{\mathrm{T}}q$, where $F = \Lambda\Gamma^{-1/2}$. In terms of these variables, one can introduce the effective potential

$$V_{\mathrm{eff}}(q) \;=\; V(q) - \tfrac{1}{2} q \cdot \Lambda\Lambda^{\mathrm{T}} q \;, \tag{2.1}$$

and the "energy" is now $G(s,q,p)$ with

$$G(s,q,p) \;=\; \tfrac{1}{2}p^2 + V_{\mathrm{eff}} + \tfrac{1}{2} s \cdot \Gamma s \;. \tag{2.2}$$

Finally, with the adjoint change in the derivatives $\nabla_q \to \nabla_q - F\nabla_s$, the equations of motion (1.9) read

$$\begin{aligned} \mathrm{d}q \;&=\; \nabla_p G \mathrm{d}t \;=\; p\,\mathrm{d}t \;, \\ \mathrm{d}p \;&=\; -(\nabla_q - F\nabla_s) G \mathrm{d}t \;=\; -\big(\nabla_q V_{\mathrm{eff}}(q) - F\Gamma s\big)\mathrm{d}t \;, \\ \mathrm{d}s \;&=\; -(\nabla_s + F^{\mathrm{T}}\nabla_p) G\,\mathrm{d}t - (2T^{1/2})\mathrm{d}w \;=\; -\big(\Gamma s + F^{\mathrm{T}} p\big)\mathrm{d}t - (2T^{1/2})\mathrm{d}w \;. \end{aligned} \tag{2.3}$$

Writing G_p for $\nabla_p G$ and G_q for $\nabla_q G$ (these are vectors with nd components), and G_s for $\nabla_s G$ (this is a vector with $2d$ components), the generator L of the diffusion process takes, in the variables $y = (s,q,p)$, the form

$$L \;=\; \nabla_s \cdot T\nabla_s - G_s \cdot \nabla_s + \big(G_p \cdot \nabla_q - G_q \cdot \nabla_p\big) + \big((FG_s)\cdot \nabla_p - G_p \cdot F\nabla_s\big) \;. \tag{2.4}$$

If f is a function on the phase space X, we let

$$S^t f(y) \;\equiv\; \big(e^{Lt} f\big)(y) \;=\; \int f\big(\xi_y(t)\big)\, d\mathbf{P}(w) \;.$$

The adjoint L^{T} of L in the space $\mathrm{L}^2(\mathbf{R}^{d(2+2n)})$ is called the Fokker-Planck operator. The density m of the invariant measure is the (unique) normalized solution of the equations $L^{\mathrm{T}} m \;=\; 0$.

2.2. The Entropy Production σ

Using the notation (2.4), we now establish a relation between the energy flux and the entropy production. Since we are dealing with a Hamiltonian setup, the energy flux is defined naturally by the time derivative of the mean evolution S^t of the effective energy, $H_{\mathrm{eff}}(q,p) \;=\; p^2/2 + V_{\mathrm{eff}}(q)$. Differentiating, we get from the equations of motion $\partial_t S^t H_{\mathrm{eff}} \;=\; S^t L H_{\mathrm{eff}}$, with

$$L H_{\mathrm{eff}} \;=\; p \cdot (-\nabla_q V_{\mathrm{eff}} + F\Gamma s) + \nabla_q V_{\mathrm{eff}} \cdot p \;=\; p \cdot F\Gamma s \;.$$

We define the total flux by $\Phi = p \cdot F\Gamma s$, and inspection of the definition of F and Γ leads to the identification of the flux at the left and right ends of the chain: $\Phi \;=\; \Phi_{\mathrm{L}} + \Phi_{\mathrm{R}}$, with

$$\Phi_{\mathrm{L}} \;=\; p_1 \cdot \Lambda_{\mathrm{L}} \Gamma_{\mathrm{L}}^{1/2} s_{\mathrm{L}} \;, \qquad \Phi_{\mathrm{R}} \;=\; p_n \cdot \Lambda_{\mathrm{R}} \Gamma_{\mathrm{R}}^{1/2} s_{\mathrm{R}} \;.$$

Note that Φ_{L} is the energy flux from the left bath to the chain, and Φ_{R} is the energy flux from the right bath to the chain. Furthermore, observe that $\langle\Phi\rangle_\mu = 0$, with $\langle f\rangle_\mu \equiv \int \mu(\mathrm{d}y)\, f(y) = \int \mathrm{d}y\, m(y) f(y)$, because $\Phi = LH_{\mathrm{eff}}$ and $L^{\mathrm{T}} m = 0$.

Since we have been able to identify the energy flux on the ends of the chain, we can *define* the (thermodynamic) entropy production σ by

$$\sigma = \frac{\Phi_{\mathrm{L}}}{T_{\mathrm{L}}} + \frac{\Phi_{\mathrm{R}}}{T_{\mathrm{R}}} = p \cdot F T^{-1} \Gamma s \,. \tag{2.5}$$

2.3. Time-Reversal, Generalized Detailed Balance Condition

We next define the "time-reversal" map J by $\big(Jf\big)(s,q,p) = f(s,q,-p)$. This map is the projection onto the space of the s,q,p of the time-reversal of the Hamiltonian flow (on the full phase space of chain plus baths) defined by the original problem (1.5).

Notation. To obtain simple formulas for the entropy production σ we write the (strictly positive) density m of the invariant measure μ as

$$m = J e^{-R} e^{-\varphi} \,, \tag{2.6}$$

where $R = R(s) = \frac{1}{2} s \cdot \Gamma T^{-1} s$. Let L^* denote the adjoint of L in the space $\mathcal{H}_\mu = \mathrm{L}^2(X, \mathrm{d}\mu)$ associated with the invariant measure μ, where $X = \mathbf{R}^{2(2n+2)}$. In terms of the adjoint L^{T} on $\mathrm{L}^2(X, \mathrm{d}s\, \mathrm{d}q\, \mathrm{d}p)$, we have the operator identity

$$L^* = m^{-1} L^{\mathrm{T}} m \,. \tag{2.7}$$

We have the following important symmetry property as suggested by the paper [10].

Theorem 2.1. *Let $L_\eta = L + \eta\sigma$, where $\eta \in \mathbf{R}$. One has the operator identity*

$$J e^{-J\varphi} (L_\eta)^* e^{J\varphi} J = L_{1-\eta} \,. \tag{2.8}$$

In particular,

$$J e^{-J\varphi} L^* e^{J\varphi} J - L = \sigma \,. \tag{2.9}$$

Remark 2.2. This relation may be viewed as a generalization to non-equilibrium of the detailed balance condition (at equilibrium, one has $JL^*J - L = 0$).

The paper of Gallavotti and Cohen [6] describes fluctuations of the entropy production. It is based on numerical experiments by [5] which were then abstracted to the general context of dynamical systems. In further work, these ideas have been successfully applied to thermostatted systems modeling non-equilibrium problems. In the papers [10] and [11] these ideas have been further extended to non-equilibrium models described by stochastic dynamics. In the context of our model, the setup is as follows: One considers the observable $W(t) = \int_0^t \mathrm{d}\eta\, \sigma\big(\xi_x(\eta)\big)$. By ergodicity, one finds $\lim_{t\to\infty} t^{-1}W(t) = \langle\sigma\rangle_\mu$, for all x and almost all realizations of the Brownian motion $\xi_x(t) = \xi_x(t,\omega)$. The rate function $\widehat{e}$ is characterized by the relation

$$\inf_{y\in I} \widehat{e}(y) \;=\; -\lim_{t\to\infty} \frac{1}{t} \log \mathbf{Prob} \left\{ \frac{W(t)}{t\langle\sigma\rangle_\mu} \in I \right\} \;.$$

Under suitable conditions it can be expressed as the Legendre transform of the function

$$e(\eta) \;\equiv\; -\lim_{t\to\infty} t^{-1} \log\big\langle e^{-\eta W(t)}\big\rangle_\mu \;.$$

Formally, $-e(\eta)$ can be represented as the maximal eigenvalue of L_η. Observing now the relation (2.8), one sees immediately that

$$e(\eta) \;=\; e(1-\eta) \;. \tag{2.10}$$

Theorem 2.3. [13] *The above relations can be rigorously justified and lead to*

$$\widehat{e}(y) - \widehat{e}(-y) \;=\; -y\langle\sigma\rangle_\mu \;. \tag{2.11}$$

In particular this means that at equal temperatures, when $\langle\sigma\rangle_\mu = 0$, the fluctuations are symmetric around the mean 0, while at unequal temperatures, the odd part is linear in y and proportional to the mean entropy production. Note that when $\langle\sigma\rangle_\mu \neq 0$ this relation describes fluctuations around 0, *not* around the mean! This is the celebrated Gallavotti-Cohen fluctuation theorem.

3. Extensions

The technique for proving uniqueness results presented above can be generalized and applied to many other problems, in particular to certain types of "partially noisy" PDE's (so that now phase space is infinite dimensional). One kind of example must suffice to illustrate the kind of results one can obtain. Consider the stochastic Ginzburg-Landau equation with periodic boundary conditions (written in Fourier components, for $L \gg 1$):

$$du_k \;=\; (1-(k/L)^2)u_k\,dt - \sum_{k_1+k_2+k_3=k} u_{k_1}u_{k_2}u_{k_3}\,dt + q_k\,dw_k \;, \quad k\in\mathbf{Z} \;, \tag{3.1}$$

with $|q_k| \sim k^{-5}$ and where w_k are standard Wiener processes. The point is here that q_k may be zero for all $|k| \le k_*$.

Theorem 3.1. [2, 8, 7] *The process defined by (3.1) has a unique invariant measure. Any initial condition is attracted exponentially fast to it.*

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